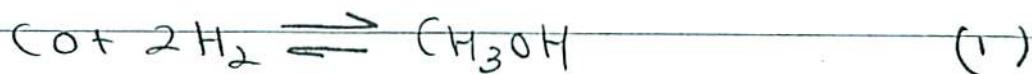


# Solution to Problem 5-3

(Problem 1-2)



Test whether system behaves as though one stoichiometrically - single reaction were taking place by applying the Law of Definite Proportions (LDP)

$$\sum (\text{extent of reaction}) = \frac{\Delta n_i}{\nu_i} = \frac{\Delta n_{\text{CO}}}{\nu_{\text{CO}}} = \frac{\Delta n_{\text{H}_2}}{\nu_{\text{H}_2}} = \frac{\Delta n_{\text{CH}_3\text{OH}}}{\nu_{\text{CH}_3\text{OH}}}$$

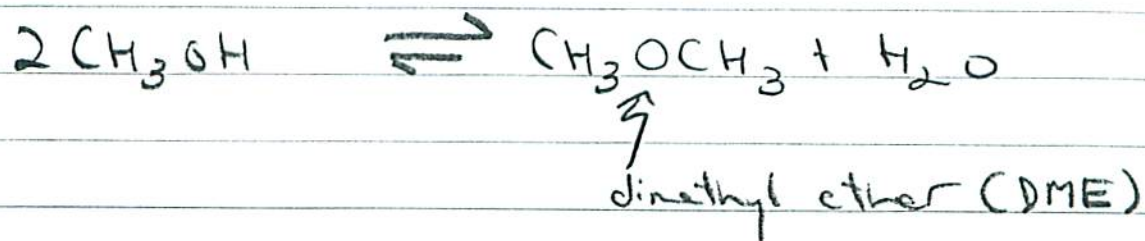
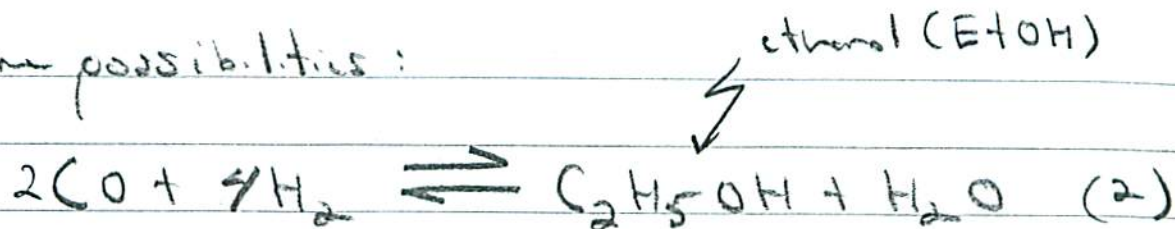
Species	$n(\text{in})$	$n(\text{out})$	$\Delta n$	$\nu_i$	$\sum$
CO	100	83	-17	-1	17
H <sub>2</sub>	72	34	-38	-2	19
CO <sub>2</sub>	9	9	0	0	-
CH <sub>4</sub>	19	19	0	0	-
CH <sub>3</sub> OH	2	13	11	+1	11

Since  $\sum$  is not the same for all species, system does not obey the LDP. Does not behave as though one "single" reaction is taking place.

Clue - amount of methanol (CH<sub>3</sub>OH) formed is less than predicted from amount of CO and H<sub>2</sub> reacted. However, CO and H<sub>2</sub> react in the proportion predicted by the above reaction.

Hypothesis - maybe another product is formed (not included in the product analysis) by the reaction of CO and H<sub>2</sub> in the ratio of 1:2

Some possibilities:



Note that both EtOH and DME have the formula  $\text{C}_2\text{H}_6\text{O}$ . The available data will not tell us which of these is formed

Suppose  $\gamma$  moles of  $\text{C}_2\text{H}_6\text{O}$  and  $\gamma$  moles of  $\text{H}_2\text{O}$  are formed as the feed passes through the reactor. Then

Species	$\Delta N$
CO	-17
$\text{H}_2$	-34
$\text{CO}_2$	-
$\text{CH}_4$	-
$\text{CH}_3\text{OH}$	+11
$\text{C}_2\text{H}_6\text{O}$	$\gamma$
$\text{H}_2\text{O}$	$\gamma$

Now, if 2 reactions are taking place, say (1) and (2), then the LDP is written as

$$\Delta N_i = \sum_j \alpha_{ij} \nu_{i,j}$$

Writing the LDP for each species

$$\Delta n_{CO} = \underline{X}_1(-1) + \underline{X}_2(-2) = -\underline{X}_1 - 2\underline{X}_2$$

$$\Delta n_{H_2} = \underline{X}_1(-2) + \underline{X}_2(-4) = -2\underline{X}_1 - 4\underline{X}_2$$

$$\Delta n_{MeOH} = \underline{X}_1(1) + \underline{X}_2(0) = \underline{X}_1 = 11$$

$$\Delta n_{EtOH} = \underline{X}_1(0) + \underline{X}_2(1) = \underline{X}_2 = \gamma$$

$$\Delta n_{H_2O} = \underline{X}_1(0) + \underline{X}_2(1) = \underline{X}_2 = \gamma$$

$$\Delta n_{CO} = -11 - 2(\gamma) = 17 \Rightarrow \gamma = 3$$

$$\Delta n_{H_2} = -2(11) - 4(\gamma) = -22 - 4(3) = -34$$

check

Hypothesis is consistent with data. (Note - data do not prove hypothesis)

To test - analyze feed and effluent for EtOH, DME, H<sub>2</sub>O and other alcohols

